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ADRIATIC INDICES AND SANSKRUTI INDEX ENVISAGE OF CARBON NANOCONE

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ABSTRACT. In [17, 18], D. Vukicevic notified the 148 discrete adriatic indices. They were analyzed on the testing sets provided by the International Academy of Mathematical Chemistry and it had been shown that they have good presaging properties in many cases. Carbon Nanocones have been observed on the surface of naturally occurring graphite and it have gained and increased scientific interest due to their unique properties and promising uses in many applications such as energy and gas storage. In this article, we frame-up with the general expression for some discrete adriatic indices and sanskruti index of Carbon Nanocones $CNC_m[n]$.

Keywords:Topological indices, adriatic indices, carbon nanocones, semi-total point graph.

AMS Subject Classification: 2000: 05C90, 05C12

1. Introduction

Molecular descriptors, being a numerical functions of molecular structure play pivotal role in mathematical chemistry. Topological indices are numerical function of an underlying molecular, represent an important types of molecular descriptors. The advantage of topological indices are they may be used directly as simple numerical descriptors in a comparison with physical, chemical or biological parameters of molecules in Quantitative Structure Property Relationships ($QSPR$) and in Quantitative Structure Activity Relationships ($QSAR$). A graph can be recognized by a numerical value, a polynomial, a sequence of numbers or a matrix representation of the graph, and these representations are aimed to be uniquely defined for that graph. There was vast research related to topological indices and its properties[5, 6].

Inspired from works of D. Vukicevic and C. K. Gupta and et al., [4, 12, 14], we deal with the certain discrete adriatic indices are shown below.

- Symmetric division deg index is a good predictor of total surface area for polychlorobiphenyls.

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- Inverse sum Indeg index is a significant predictor of total surface area for octane isomers
- Misbalance type deg indices (such as Misbalance lodeg index, Misbalance rodeg index, Misbalance hadeg index, Misbalance irdeg index, Misbalance deg index and Misbalance losdeg) are the best predictor of standard enthalpy of vaporisation for octane isomers
- Inverse sum losdeg index is the best predictor of heat capacity at constant P and of total surface area for octane isomers.

Another most succesful index named as Augmented zagreb index, it is useful for computing the heat of formation of alkanes.

Recently, Hosamani [8] put forward a novel topological index, namely the sanskruti index of a molecular graph G, it gives good correlation with entropy of an octane isomers.

In 1994, Ge and Sattler [3] found carbon nanocones (CNC) and carbon nanostructures have attracted considerable attention due to their potential use in many applications including energy storage, gas sensors, biosensors, nanoelectronic devices and chemical probes [9]. Carbon allotropes such as carbon nanocones and carbon nanotubes have been proposed as possible molecular gas storage devices. Nowadays nanostructues involving carbon have been the focus of an intense research activity. One can see [2, 7, 10, 19] for relevant work on carbon nanomaterials. For more attention on the topological indices may refer,[11, 16].

This article, dealt with three sections. In section 1 surrounds introduction, followed by essential prerequisite results in section 2 and final section concentrated with main results.

2. Essential prerequisite

In this section, we recall some essential definitions and discuss prerequisites useful to development of the article.

Definition 2.1. [8] *Let G be a graph and Sanskruti index of G is a graph and degree of every vertex is sum of the degree of the neighborhood vertices i.e., $S_u = \sum_{uv} d_v$ and is defined as*

$$\mathcal{S}(G) = \sum_{uv \in E(G)} \left[\frac{S_u S_v}{S_u + S_v - 2} \right]^3$$

Definition 2.2. [1, 13] *Let G be graph and $R(G)$ is the semi-total point graph of G obtained from G by adding a new vertex corresponding to each edge of G and by joining each new vertex to the end vertices of the edge corresponding to it.*

Let G be a graph and d_u is a degree of vertex $u \in V(G)$, then Adriatic indices as defined below table.

Logarithm of modified first multiplicative zagreb index	$\overline{LM_1}(G) = \sum_{uv \in E(G)} ln\left[d_u + d_v\right]$
Misbalance lodeg index	$MLD(G) = \sum_{uv \in E(G)} \mid lnd_u - lnd_v \mid$
Misbance rodeg index	$MRD(G) = \sum_{uv \in E(G)} \mid \sqrt{d_u} - \sqrt{d_v} \mid$
Misbalance haddeg index	$MHD(G) = \sum_{uv \in E(G)} \mid 2^{-d_u} - 2^{-d_v} \mid$
Misbalance irdeg index	$MIRD(G) = \sum_{uv \in E(G)} \mid \frac{1}{\sqrt{d_u}} - \frac{1}{\sqrt{d_v}} \mid$
Misbalance deg index	$MD(G) = \sum_{uv \in E(G)} \mid d_u - d_v \mid$
Misbalance losdeg index	$MLSD(G) = \sum_{uv \in E(G)} \mid ln^2 d_u - ln^2 d_v \mid$
Inverse sum los-deg index	$ISLSD(G) = \sum_{uv \in E(G)} \left[\frac{1}{\sqrt{lnd_u} + \sqrt{lnd_v}}\right]$
Sanskruti index	$\mathcal{S}(G) = \sum_{uv \in E(G)} \left[\frac{S_u S_v}{S_u + S_v - 2}\right]^3$

The graphical structure of $CNC_m[n]$ nanocones [15] have a cycle of m-length at its central part and n-levels of hexagons positioned at the conical exterior around its central part. The graph of $CNC_m[n]$, where $m \geq 3, n = 1, 2, 3, ...$ has $\frac{m(n+1)(3n+2)}{2}$ edges and $m(n+1)^2$ vertices and is shown in Figure 1.

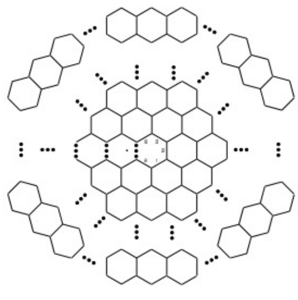

Figure 1: $CNC_k[n]$

Table 1: The edge partition of carbon nanocone $CNC_m[n]$ based on degrees of end vertices of each edge.

Number of edges	(d_u, d_v) where $uv \in E(G)$
m	(2,2)
$\frac{mn(3m+1)}{2}$	(3,3)
$2mn$	(3,2)

Table 2: The edge partition of carbon nanocone $CNC_m[n]$ based on degree sum of neighbourhood vertices of end vertices of each edge.

Number of edges	(S_u, S_v) where $uv \in E(G)$
m	(5,5)
$2m$	(5,7)
$m(2n-2)$	(6,7)
mn	(7,9)
$\frac{mn}{2}(3n-1)$	(9,9)

Lemma 2.1. [1] *Let G be graph with n vertices and m edges, then graph $R[G]$ has $(n+m)$ vertices and $3m$ edges.*

Table 3: The edge partition of semi-total point graph of carbon nanocone $R[CNC_m[n]]$ based on degrees of end vertices of each edge.

Number of edges	(d_u, d_v) where $uv \in E(G)$
$2m(n+1)$	(2,4)
m	(4,4)
$3mn(n+1)$	(2,6)
$2mn$	(4,6)
$\frac{mn}{2}(3n+1)$	(6,6)

3. Main Results

This section dealt with results related ISI, AZI, SDD, LM_1,$\overline{LM_1}$, MLD, MRD, MHD, $MIRD$, MD, $MLSD$, $ISLSD$ and Sanskruti index of carbon nanocone.

Theorem 3.1. *Let G be a graph of $CNC_m[n]$ nanocones for $m \geq 3$ and $n = 1, 2, 3, \ldots$. Then*

$$\begin{aligned} ISI[G] &= \tfrac{m}{20}[45n^2 + 27n + 20]. \\ AZI[G] &= 8m + \tfrac{3^6}{2^7}mn(3n+1) + 16mn. \\ SDD[G] &= m\left[2 + n\left(3n + \tfrac{16}{3}\right)\right]. \end{aligned}$$

Proof. The graph G consists of $m(n+1)^2$ vertices and $\frac{m(n+1)(3n+2)}{2}$ edges as shown in fig 1. Using table 1 we obtain the results as follows.

$$\begin{aligned} ISI[G] &= m\left[\tfrac{2.2}{2+2}\right] + \tfrac{mn(3n+1)}{2}\left[\tfrac{3.3}{3+3}\right] + 2mn\left[\tfrac{3.2}{3+2}\right]. \\ &= \tfrac{m}{20}[45n^2 + 27n + 20]. \\ AZI[G] &= m\left[\tfrac{2.2}{2+2-2}\right]^3 + \tfrac{mn(3n+1)}{2}\left[\tfrac{3.3}{3+3-2}\right]^3 + 2mn\left[\tfrac{3.2}{3+2-2}\right]^3. \\ &= 8m + \tfrac{3^6}{2^7}mn(3n+1) + 16mn. \\ SDD[G] &= m\left[\tfrac{2^2+2^2}{2.2}\right] + \tfrac{mn(3n+1)}{2}\left[\tfrac{3^2+3^2}{3.3}\right] + 2mn\left[\tfrac{3^2+2^2}{3.2}\right]. \\ &= m\left[2 + n\left(3n + \tfrac{16}{3}\right)\right]. \end{aligned}$$

□

Theorem 3.2. *Let G be a graph of $CNC_m[n]$ nanocones for $m \geq 3$ and $n = 1, 2, 3, \ldots$. Then*

$$\begin{aligned} LM_1[G] &= 2m\left[ln2 + \tfrac{n(3n+1)}{3}ln3 + \tfrac{n}{3}[ln72]\right]. \\ \overline{LM_1}[G] &= ln[4.(6)^{\frac{n(3n+1)}{2}} 5^{2n}]^m. \\ MLD[G] &= 2mn|ln(\tfrac{3}{2})|. \\ MLSD[G] &= 2mn|ln^2 3 - ln^2 2|. \end{aligned}$$

Proof. The graph G consists of $m(n+1)^2$ vertices and $\frac{m(n+1)(3n+2)}{2}$ edges as shown in fig 1. Using table 1 we obtain the results as follows.

$$\begin{aligned} LM_1[G] &= 2m\left[\tfrac{ln2}{2} + \tfrac{ln2}{2}\right] + 2\left[\tfrac{mn(3n+1)}{2}\right]\left[\tfrac{ln3}{3} + \tfrac{ln3}{3}\right] + 2(2mn)\left[\tfrac{ln2}{2} + \tfrac{ln3}{3}\right]. \\ &= 2m\left[ln2 + \tfrac{n(3n+1)}{3}ln3 + \tfrac{n}{3}[ln72]\right]. \\ \overline{LM_1}[G] &= m[ln(2+2)] + \tfrac{mn(3n+1)}{2}[ln(3+3)] + 2mn[ln(3+2)]. \\ &= ln[4.(6)^{\frac{n(3n+1)}{2}} 5^{2n}]^m. \\ MLD[G] &= m|ln2 - ln2| + \tfrac{mn(3n+1)}{2}|ln3 - ln3| + 2mn|ln3 - ln2|. \\ &= 2mn|ln\left(\tfrac{3}{2}\right)|. \\ MLSD[G] &= m|ln^2 2 - ln^2 2| + \tfrac{mn(3n+1)}{2}|ln^2 3 - ln^2 3| + 2mn|ln^2 3 - ln^2 2|. \\ &= 2mn|ln^2 3 - ln^2 2|. \end{aligned} \tag{1}$$

□

Theorem 3.3. *Let G be a graph of $CNC_m[n]$ nanocones for $m \geq 3$ and $n = 1, 2, 3, \ldots$. Then*

$$\begin{aligned} MRD[G] &= 2mn|\sqrt{3} - \sqrt{2}|. \\ MIRD[G] &= 2mn|\tfrac{1}{\sqrt{3}} - \tfrac{1}{\sqrt{2}}|. \\ ISLSD[G] &= m\left[\tfrac{1}{2\sqrt{2}}\right] + \tfrac{mn(3n+1)}{2}\left[\tfrac{1}{2\sqrt{3}}\right] + 2mn\left[\tfrac{1}{\sqrt{3}+\sqrt{2}}\right]. \end{aligned}$$

Proof. The graph G consists of $m(n+1)^2$ vertices and $\frac{m(n+1)(3n+2)}{2}$ edges as shown in fig 1. Using table 1 we obtain the results as follows.

$$\begin{aligned} MRD[G] &= m|\sqrt{2} - \sqrt{2}| + \tfrac{mn(3n+1)}{2}|\sqrt{3} - \sqrt{3}| + 2mn|\sqrt{3} - \sqrt{2}|. \\ &= 2mn|\sqrt{3} - \sqrt{2}|. \\ MIRD[G] &= m|\tfrac{1}{\sqrt{2}} - \tfrac{1}{\sqrt{2}}| + \tfrac{mn(3n+1)}{2}|\tfrac{1}{\sqrt{3}} - \tfrac{1}{\sqrt{3}}| + 2mn|\tfrac{1}{\sqrt{3}} - \tfrac{1}{\sqrt{2}}|. \\ &= 2mn|\tfrac{1}{\sqrt{3}} - \tfrac{1}{\sqrt{2}}|. \\ ISLSD[G] &= m\left[\tfrac{1}{\sqrt{2}+\sqrt{2}}\right] + \tfrac{mn(3n+1)}{2}\left[\tfrac{1}{\sqrt{3}+\sqrt{3}}\right] + 2mn\left[\tfrac{1}{\sqrt{3}+\sqrt{2}}\right]. \\ &= m\left[\tfrac{1}{2\sqrt{2}}\right] + \tfrac{mn(3n+1)}{2}\left[\tfrac{1}{2\sqrt{3}}\right] + 2mn\left[\tfrac{1}{\sqrt{3}+\sqrt{2}}\right]. \end{aligned}$$

□

Theorem 3.4. *Let G be a graph of $CNC_m[n]$ nanocones for $m \geq 3$ and $n = 1, 2, 3, \ldots$. Then*

$$\mathcal{S}[G] = \left[\tfrac{81}{16}\right]^3 + mn\left[\tfrac{9}{2}\right]^3 + m\left[\tfrac{25}{8}\right]^3 + 2m\left[\tfrac{7}{2}\right]^3 + m(2n-2)\left[\tfrac{42}{11}\right]^3.$$

Proof. The graph G consists of $m(n+1)^2$ vertices and $\frac{m(n+1)(3n+2)}{2}$ edges as shown in fig 1. Using table 2 we obtain the results as follows.

$$\begin{aligned}\mathcal{S}[G] &= \tfrac{mn}{2}(3n-1)\left[\tfrac{9.9}{9+9-2}\right]^3 + mn\left[\tfrac{7.9}{7+9-2}\right]^3 + m\left[\tfrac{5.5}{5+5-2}\right]^3 + 2m\left[\tfrac{5.7}{5+7-2}\right]^3 + m(2n-2)\left[\tfrac{6.7}{6+7-2}\right]^3. \\ &= \left[\tfrac{81}{16}\right]^3 + mn\left[\tfrac{9}{2}\right]^3 + m\left[\tfrac{25}{8}\right]^3 + 2m\left[\tfrac{7}{2}\right]^3 + m(2n-2)\left[\tfrac{42}{11}\right]^3.\end{aligned}$$

□

Theorem 3.5. *Let G be a graph of $R[CNC_m[n]]$ nanocones for $m \geq 3$ and $n = 1, 2, 3, \ldots$. Then*

$$\begin{aligned}ISI[G] &= m\left[9n^2 + \tfrac{359}{30} + \tfrac{37}{6}\right]. \\ SDD[G] &= m\left[24n^2 + \tfrac{526}{15}n + \tfrac{32}{3}\right].\end{aligned}$$

Proof. The graph G consists of $\frac{m(n+1)(5n+4)}{2}$ vertices and $\frac{3m}{2}(n+1)(3n+2)$ edges by lemma 2.1. Using table 3 we obtain the results as follows.

$$\begin{aligned}ISI[G] &= 2m(n+1)\left[\tfrac{2.4}{2+4}\right] + m\left[\tfrac{4.4}{4+4}\right] + 3mn(n+1)\left[\tfrac{2.6}{2+6}\right] + 2mn\left[\tfrac{4.6}{4+6}\right] + \tfrac{mn}{2}(3n+1)\left[\tfrac{6.6}{6+6}\right]. \\ &= m\left[9n^2 + \tfrac{359}{30} + \tfrac{37}{6}\right]. \\ SDD[G] &= 2m(n+1)\left[\tfrac{2^2+4^2}{2+4}\right] + m\left[\tfrac{4^2+4^2}{4+4}\right] + 3mn(n+1)\left[\tfrac{2^2+6^2}{2+6}\right] + 2mn\left[\tfrac{4^2+6^2}{4+6}\right] + \tfrac{mn}{2}(3n+1)\left[\tfrac{6^2+6^2}{6+6}\right]. \\ &= m\left[24n^2 + \tfrac{526}{15}n + \tfrac{32}{3}\right].\end{aligned}$$

□

4. CONCLUSIONS

In this paper, we reclaimed thirteen degree based topological indices of carbon nanocone. We have used the algebraic method i.e., edge partition method for these compounds to compute the general expression. It is clear that, these results have benefits to forecast the physical properties of elemental chemical compounds for example discrete adriatic indices is useful for determining the physio-chemical properties of alkanes as remarked by D. Vukicevic and his co-workers. He noticed that there is perfect correlation between discrete adriatic indices and polychlorobiphenyls, octane isomers .

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